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Deployment of a Continuously Operated µChemLab[TM]

Richard Kottenstette, Patrick Lewis, Douglas R. Adkins, George R. Dulleck, Jr., Greg Foltz, Susanna Gordon and Michael Oborny

Prepared by
Sandia National Laboratories
Albuquerque, New Mexico 87185 and Livermore, California 94550

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Richard Kottenstette, Patrick Lewis and Douglas R. Adkins,
Micro Analytical Systems Department
Sandia National Laboratories

George R. Dulleck Jr.
Integrated Microsystems Department

Michael Oborny
ES&H Support Department

Susanna Gordon and Greg Foltz
Systems Research Department

Sandia National Laboratories
P.O.Box 5800
Albuquerque, NM 87185-0892

Abstract

A continuously operating prototype chemical weapons sensor system based on the µChemLab™ technology was installed in the San Francisco International Airport in late June 2002. This prototype was assembled in a National Electric Manufacturers Association (NEMA) enclosure and controlled by a personal computer collocated with it. Data from the prototype was downloaded regularly and periodic calibration tests were performed through modem-operated control. The instrument was installed just downstream of the return air fans in the return air plenum of a high-use area of a boarding area. A CW Sentry, manufactured by Microsensor Systems, was installed alongside the µChemLab unit and results from its operation are reported elsewhere. Tests began on June 26, 2002 and concluded on October 16, 2002. This report will discuss the performance of the prototype during the continuous testing period. Over 70,000 test cycles were performed during this period. Data from this first field emplacement have indicated several areas where engineering improvements can be made for future field emplacement.

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Thanks to the staff at San Francisco International Airport for site support and facilitation of testing.

Introduction

Chemical Sensor Requirements

One objective of the Program Response Options and Technology Enhancements for Chemical/Biological Terrorism (PROTECT) program, funded by the Chemical and Biological National Security Program of the DOE, is to investigate how a chemical or biological agent would spread inside of a subway or airport terminal. The airport program is now referred to as Protective and Responsive Options for Airport Counter-Terrorism (PROACT). In conjunction with this program a continuously operated prototype based on the µChemLab™ technology was placed in an air-handling plenum at the San Francisco International Airport. Appendix 1 gives design and operational guidance for detectors that will be used as part of an early warning detector for facilities protection.

Description of the µChemLab™

The µChemLab [1-3] consists of a miniature gas chromatographic system that uses

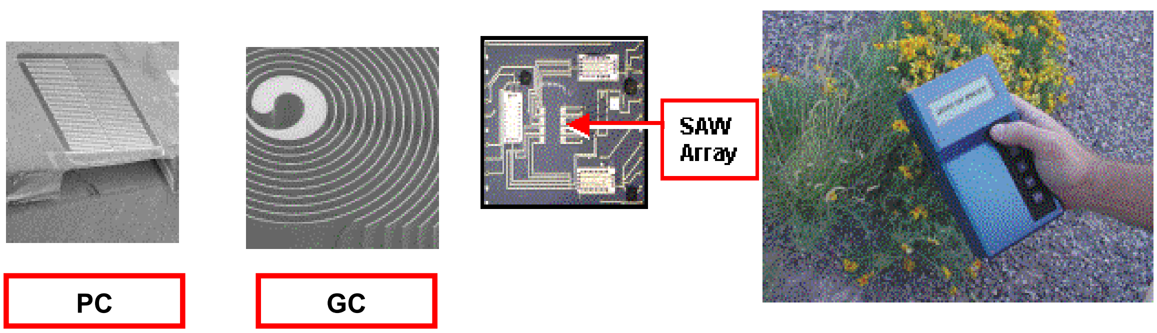

Figure 1. Microfabricated Elements of Hand-held Analyzer

microfabricated components to sample, separate and detect airborne chemicals. These components are shown in Figure 1 and include a microfabricated preconcentrator (PC), a chip-based gas chromatographic (GC) column and an array of small surface acoustic wave (SAW) devices for detection. The complete system shown on the far right in Figure1 also has other components such as a small diaphragm pump, a sampling valve and a microprocessor with an LCD display. The portable system also has a battery pack but does not have active temperature control circuitry and provides analysis on demand rather than continuously. The overall size of the portable analyzer is 8” x 4” x 2”. This system has been used at Edgewood Chemical and Biological Center and the Nevada Test Site for lab and field-testing with chemical weapons vapors and simulants.

Continuously Operated Prototype

The continuously operated prototype has been specially designed to ignore common volatile chemicals that result from industrial and maintenance activities and to detect chemical warfare vapors including both nerve and blister agents. This analyzer has also been fitted with an internal calibration module that can deliver a known quantity of a test compound to verify the systems performance. Prior to testing in the San Francisco Airport the instrument was laboratory tested in a semi continuous fashion and logged over 12000 runs.

The hardware for the PROTECT (or continuously operated µChemLab™) prototype is quite different from the portable µChemLab™. The box is much larger (NEMA box 14"x16"x8") in order to include an internal temperature-controlled chamber (insulated) in which the electronics and analytical elements reside. Additionally, the continuously operated prototype has a customized self-test feature that allows the operator to open a valve to a metered sample of nerve agent simulant dimethyl methyl phosphonate (DMMP) to challenge the system. The self-test hardware including the internal standard (IS) is shown in Figure 2.

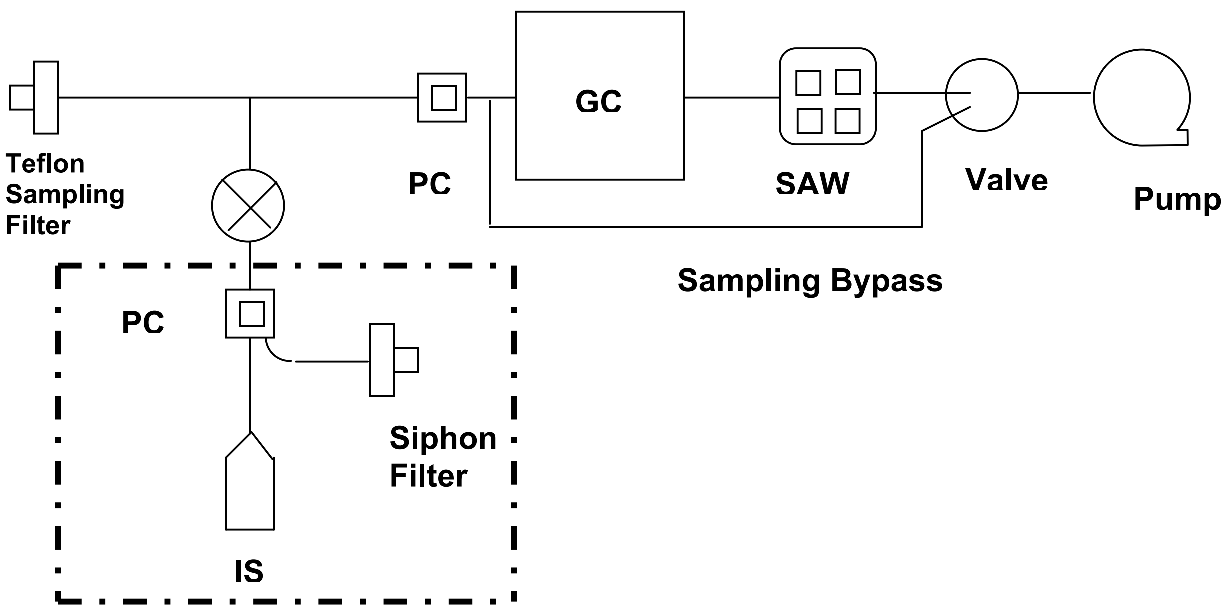

Figure 2. µChemLab™ Component Parts - Including Self-test Hardware for Continuous Operation (shown in dotted box).

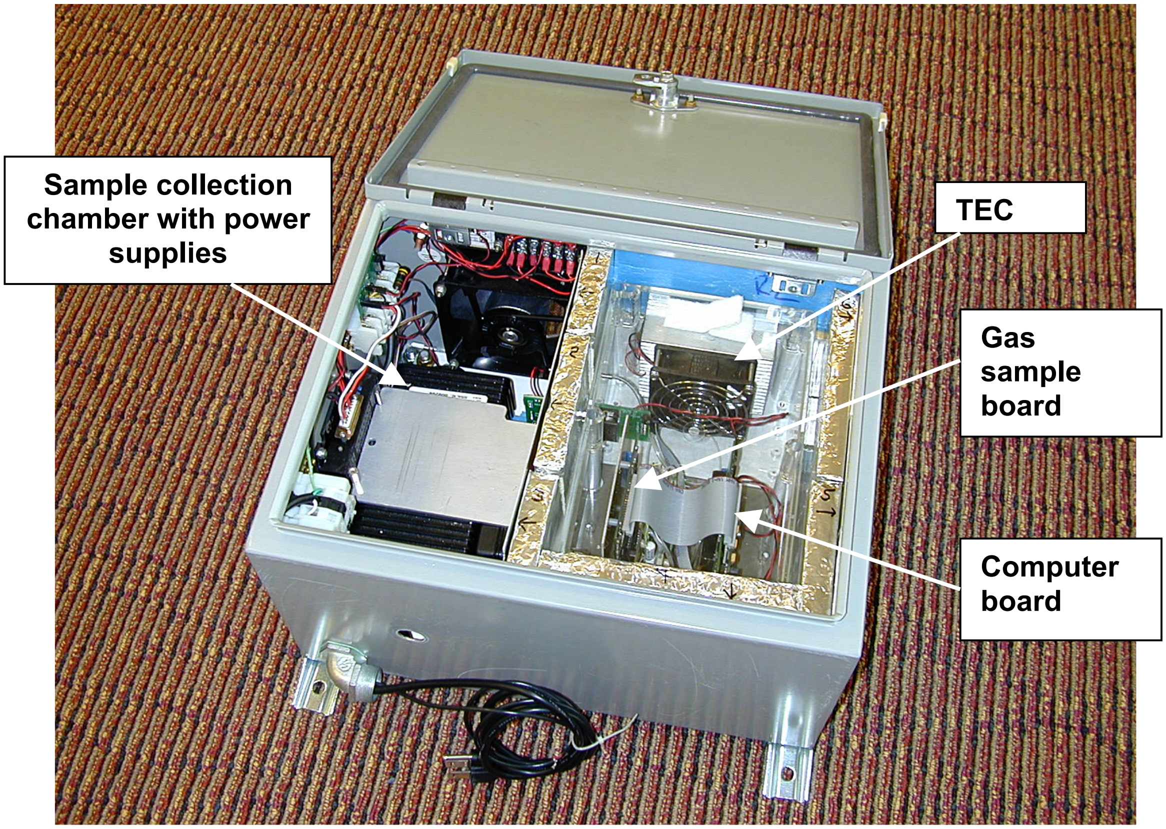

Figure 3. Continuously Operated Prototype (PROTECT)

The instrument pictured in Figure 3 consists of two compartments; the first is a sampling chamber where outside air is pulled into the box using a fan. This chamber also contains two power supplies, one for the thermoelectric controller (thermal pile - TEC) and one for the electronics along with various bus bars. The second chamber houses the gas analysis board that includes the microfabricated preconcentrator, a planar micro gas chromatograph and a surface acoustic wave array detector. A diaphragm pump is used to pull sample from the sampling chamber through a Teflon filter into the gas module and across the microfabricated preconcentrator during sampling. One of the key requirements for the PROTECT program is to have an analysis every two minutes for 24 hours a day and the prototype performs to this specification. After a sampling period of 60 seconds a three way valve located on the gas board switches to analyze the collected sample from the preconcentrator. When the valve is switched the gas chromatograph and SAW array are in-line with the preconcentrator and the diaphragm pump pulls air carrier gas across the entire analytical train (PC, GC, SAW). The preconcentrator is heated rapidly to 200°C to thermally inject the sample into the GC column. The sample is separated in the GC column while a thermal ramp is applied to the column and the separated components elute from the column into the SAW array. As different components emerge from the column they partition into the polymer zones that are deposited in the SAW delay line path. The chromatographic separation and detection takes 47 seconds. Each chemical sorbs into the polymer and dampens the surface acoustic wave to give a phase change that is measured using on-board application specific integrated circuit (ASIC). The gas-sensing module is temperature controlled with a thermoelectric device (TE Technologies AC-027) thermostatted to control instrument drift. Figure 4 shows the self-test hardware including the silver sample reservoir, preconcentrator fixture, siphon filter and solenoid valve. The right side of Figure 4 shows a close up of the diffusion source next to the sample reservoir and preconcentrator membrane while the left side shows the assembly mounted to the back of the electronics support board, as used in the PROTECT box.

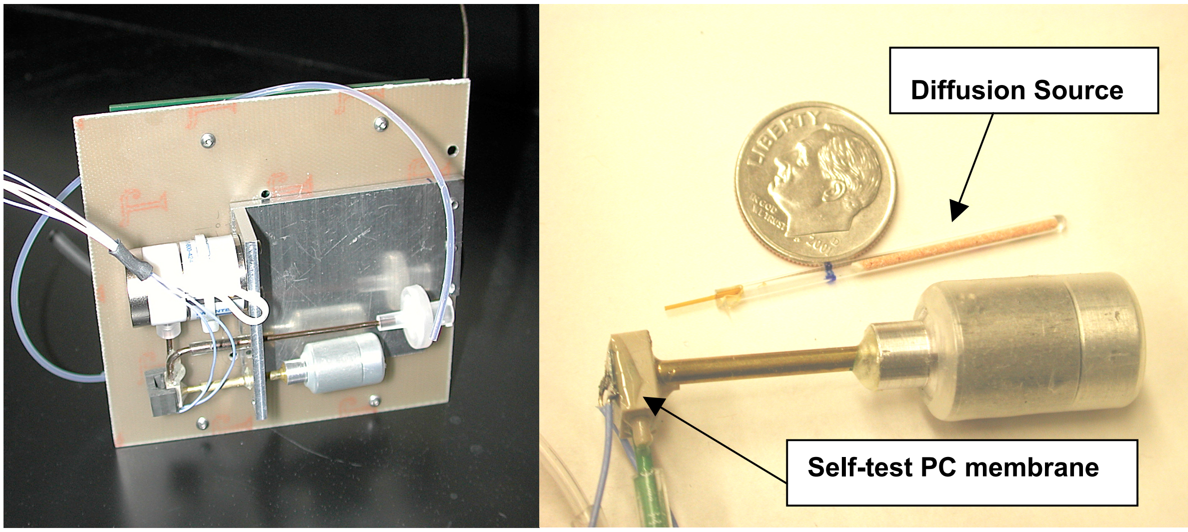

Figure 4. Self-test Assembly with Close up of Diffusion Source and Self-test Preconcentrator

Electronic Hardware

Appendix 2 contains three diagrams that describe the PROTECT box operation and control. Figure 2-1 shows a state diagram for the analyzer, Figure 2-2 shows a high-level code diagram and Figure 2-3 shows operational code and messages for the analyzer. The PROTECT electronics are based on the current μChemLab design but have several modifications to provide for additional measurements and for a controlled temperature box in which the electronics and gas module reside.   Figure 4 compares the basic μChemLab electrical blocks to those used by PROTECT.

The base firmware used in PROTECT and μChemLab is the same (since they have the same micro controller and electronics board), however, there are several major additions to the "outer control loop" in the PROTECT system.

The μChemLab code (firmware) is written to be used by an operator where commands are issued either by the local keyboard or from a RS-232 input. The box has very little in the way of problem determination since the user is present at all times.   The keyboard commands are basic and allow the operator to start and stop a run and to display the results of the last analysis. The RS-232 input allows many additional commands related to operational testing as well as determining the type of output, which will come from the RS-232 port when a run is being performed. The output data may be used to generate a chromatograph either in real time or via stored data.

The PROTECT box firmware is based on the µChemLab code but has a more complicated outer control loop which includes additional controls and tests to determine if the box is operating properly. Since PROTECT is run remotely there is no local display or keyboard and all control is either automatic or through RS-232 input. Unlike µChemLab the output of the PROTECT system is by a message system which indicates a CLEAR or ALERT condition. If an ALERT is generated, then concentrations of the specific analytes being detected are also indicated. In both instances, additional data is also transmitted which indicates box operational status. The last 30 sets of chromatographic data are also stored in the box and require remote readout if detailed information is desired. Operations codes and message formats are listed in appendix A.

By temperature controlling the prototype there was great improvement in response uniformity, increased reliability of components (no temperature cycling).The system can now operate over a wider temperature range than the portable µChemLab. The temperature is controlled by a system, which has its own controller and power supply. The TEC can be run at a variety of temperatures and for humid environments can be set to minimize dewing. Testing of the PROTECT box was performed in the environmental test facility at Sandia National Laboratories over the range of –10°F to +100°F at up to 80% humidity.

Experimental Setup Both the Sandia prototype and the CW Sentry are shown in Figure 5 next in the return-air-handling duct in front of a set of louvers (closed in the picture) for regulating exhaust of return air. AC Power was available for the test setup. A field-hardened laptop (Panasonic Toughbook) was installed with the two analyzers and connected by telephone modem for control and readout using remote operating software (PC Anywhere). A stainless steel sampling tube was installed on each box to extend into the high velocity stream coming from the return fan. All cables and components were taped to the floor of the plenum since the airflow during operation is quite high. After installation and checkout the door isolating the plenum was closed and the air system was restarted. The force of the wind exiting the duct could be seen moving the sampling tubes slightly back and forth. After installation the instrument was remotely controlled using a modem connection to the PC and the command set delineated in Appendix 3. Self-tests were performed on an intermittent basis to check peak retention time, peak amplitude and a variety of operational parameters.

Testing Results

Over the five month testing period, no false positive results were encountered. Self-tests were run periodically to test the operational performance of the analyzer. Figure 6 shows an example of a self-test chromatogram. This chromatogram shows two successive runs and is typical of a properly functioning self-test. The signal designated as "memory" represents left over sample that must be cleared out of the system. This second trace will result in a second alarm, but is always associated with a self-test event and can be discounted for this reason. Self-tests can be run in the middle of the night to establish system readiness and yet not affect performance during hours when travelers are present.

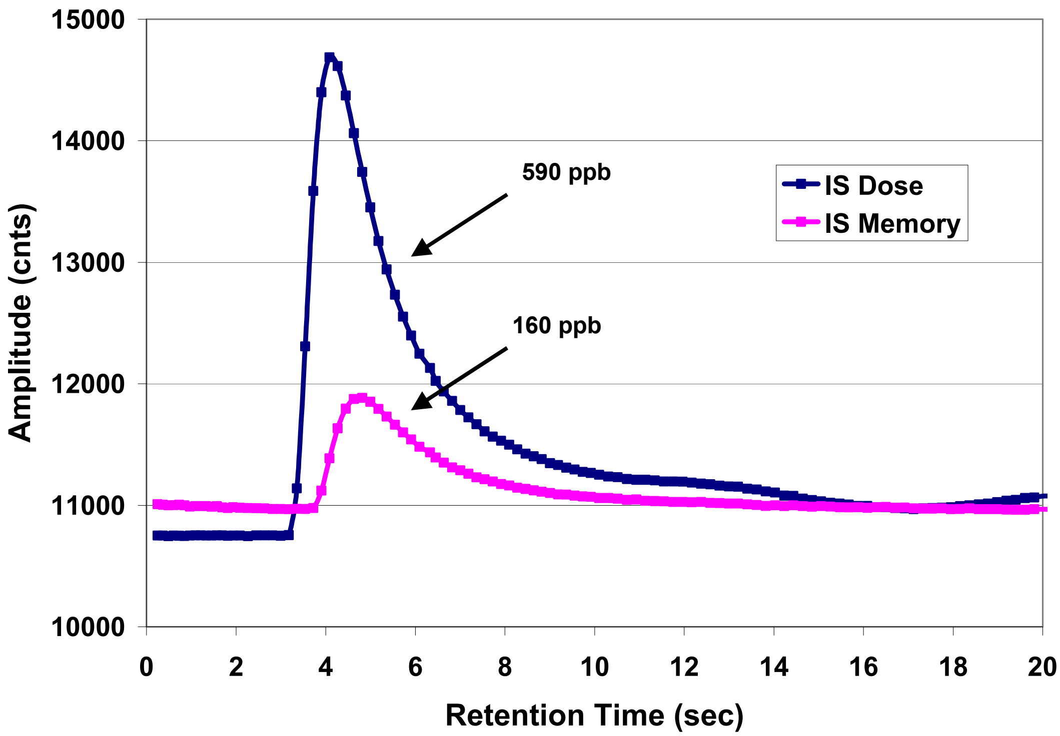

Figure 6. Self-test Chromatogram Including Subsequent Test

Data from the self-tests was recorded and is tabulated in Table 1. During a self-test cycle several key operational parameters (box temperature, pump pressure and relative humidity) are measured and a valve is opened to desorb an internal standard aliquot into the analyzer. Box temperature readings showed that the thermal electric cooler performed well and kept the analyzer at an even temperature throughout the testing. Outside of the temperature controlled region of the analyzer the temperature varied along with ambient conditions. Self-test vapor phase concentrations were measured using customized peak search and analysis software.

Table 1: San Francisco Airport Testing Summary for the PROTECT Box from June 2002 till October 2002.

Date	Time	Detection (ppb)	Retention Time (sec)	Pump** Pres.	Box Temp (°C)	RH (%)
6/28/2002	10:28	330*	5.18	44770	39	
7/3/2002	20:38	82*	5.36	44474		
7/6/2002	7:17	na*	na	44522	39	
7/9/2002	14:44	0*	0(5.37)	44660	39	
7/9/2002	15:07	99*	3.73(5.36)	44719		
7/10/2002	13:46	500	5.37	44692	39	
7/11/2002	13:43	500	5.55	44767	39	
7/12/2002	14:07	500	5.54	44690	39	45
7/14/2002	15:20	500	5.55	44698	39	43
7/16/2002	14:50	490	5.54	45164	39	44
7/18/2002	13:32	490	5.54	44984	39	46
7/22/2002	21:15	460	5.54	45168	39	44
7/24/2002	20:48	450	5.55	44751	39	43
7/29/2002	8:21	420	5.72	44832	39	46
8/4/2002	20:26	380	5.73	45141	39	44
8/6/2002	14:47	350	5.73	45158	39	40
8/9/2002	16:21	340	5.73	45557	39	21
8/13/2002	13:47	330	5.91	45909	39	46
8/14/2002	14:04	300	5.92	45612	39	47
8/16-27/02	system down time					
8/27/2002	16:39	240	6.10	45632	39	35
9/2/2002	18:35	230	5.73	45866	39	37
9/7/2002		200				
9/18/2002	19:57	140	6.83	45909	38	40
9/25/2002	15:25					
9/30/2002	15:38	50	7.51	45928	38	42
10/3/2002	9:10	40	8.60	45933	38	30
10/06/2002	14:25	40	9.14	46036	37	37

- *Phase condition for SAW device relatively nonlinear due to phase rollover. Dither signal to return to linear calibration on 7/9/02.
- * * Pump pressure is reported in A/D counts and indicates that pump function was normal throughout the testing.

Retention times and concentrations were recorded in Table 1. A self-test is designed to alarm the system and this proved to be the case. Alarms were generated for each self-test with the exception of 7/3/02 to 7/9/02. Testing during the first few days (from 6/28/02 to 7/9/02) showed low detections for the internal standard since the SAW array was exhibiting a phase rollover condition that yields nonlinear results. A feature of the software/hardware is the ability to correct this condition by dithering the signal. The SAW sensor was dithered on 7/9/02 to return to a linear phase condition and subsequent analyses showed excellent

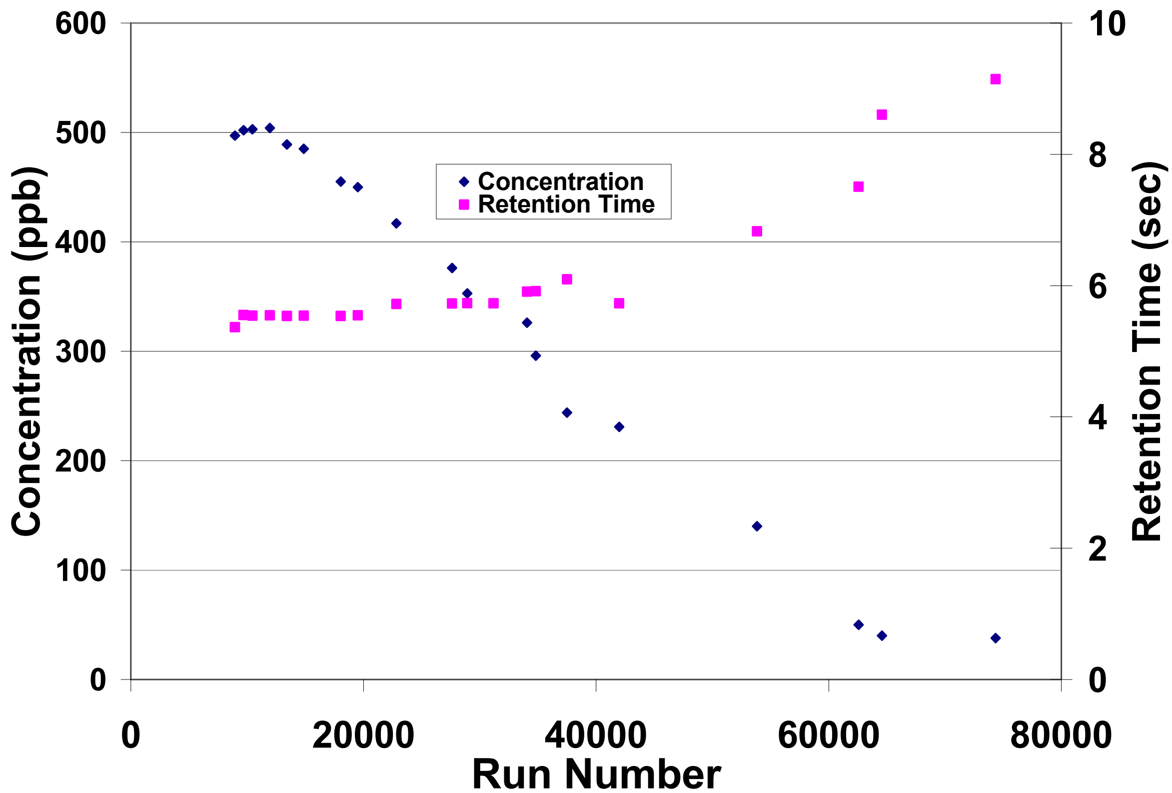

Figure 7. Composite Results from Self-test Diagnostic June-October 2002

reproducibility of the chemical challenge. Results from Table 1 are presented in Figure 7 and reveal a slow and steady decrease in the measured DMMP concentration. This drop off in sensitivity is due to a few factors including slight plugging of the Teflon filter in the sampling port and a leak that developed at a gas chromatographic column interface. Both issues are discussed in the Hardware Analysis Section.

Figure 8 shows a composite plot of chromatograms for the self-test diagnostic test. These results corroborate the quantitative results in Figure 7. The composite chromatograms indicate a shift in retention time and a lowering of peak height as the signal degrades over time. Electronic testing revealed that the loss of peak height and essential "broadening" of the signal pointed to a fluidic problem. In order to document the effect it was decided to allow the test to conclude in late October.

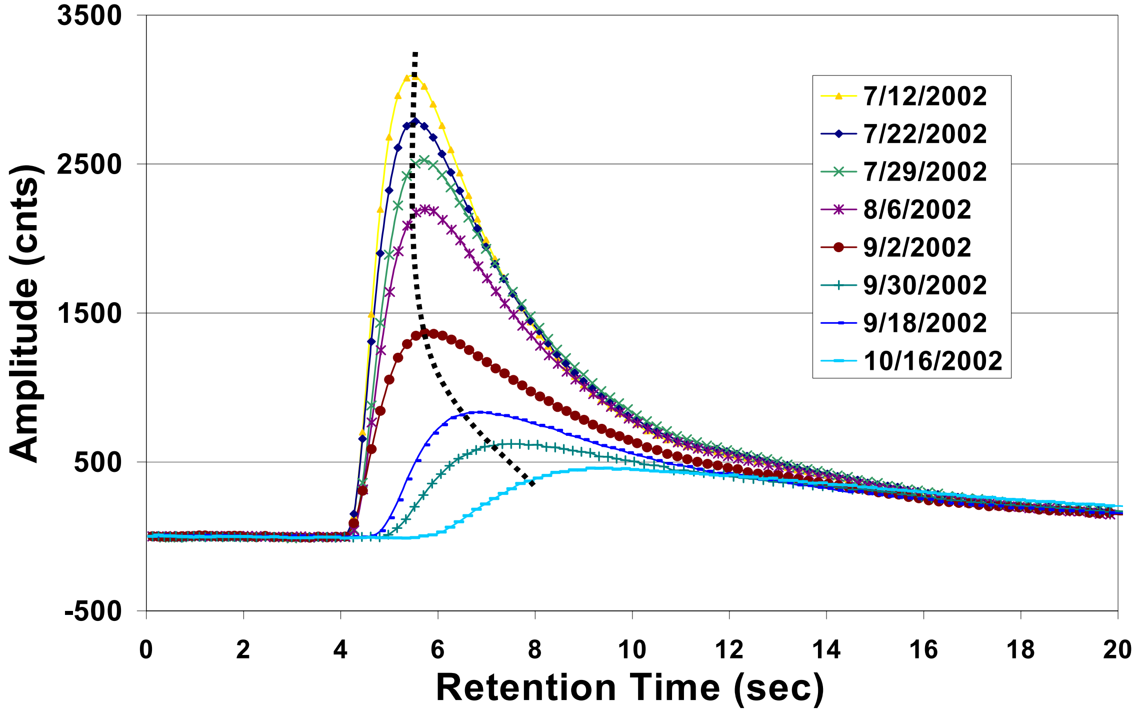

Figure 8. Chromatograms from Self-test Diagnostic July-October 2002

Hardware Analysis

After the analyzer was shipped back to Albuquerque a series of tests were run to determine the cause of the loss of performance. Figure 3 shows the sample chamber on the left side of the analyzer. Air is continuously drawn into this chamber with a muffin fan at a rate of approximately 10 cubic feet/min. Sample air is taken into the microfabricated analyzer through a small Teflon sampling filter (shown in Figure2) by

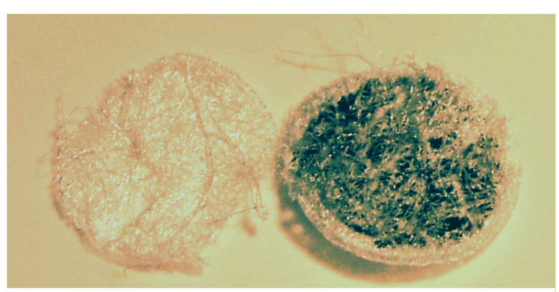

Figure 9. Whatman 1.0µm, 13mm dia. PTFE filter (new-used)

means of a small diaphragm pump that pulls the sample through the entire analysis channel. The sample filter on the box was slightly discolored due to build up of dust. Later analysis of the dust showed that a portion of it looked like fiber, possibly from carpets and fabrics from the terminal that were entrained in the return air. Figure 9 shows a picture of a new filter next to the used filter with obvious discoloration.

Table 2. Flow Testing of Clean and Used Sample Filters

PROTECT Box filter*			New Filter**		
pressure (bar)	psi	flow (mL/min)	pressure (bar)	psi	flow (mL/min)
0.02	0.29	163	0.02	0.29	275
0.04	0.58	182	0.04	0.58	1293
0.06	0.87	213	0.06	0.87	1350
0.08	1.16	237	0.08	1.16	1440
0.1	1.45	250	0.1	1.45	1500
0.12	1.74	290	0.12	1.74	1540

*In box bypass flow was 105 mL/min,
** In box bypass flow was 215 mL/min

Table 2 shows results from flow testing of the filters shown in Figure 9. Nitrogen pressure was applied to the filter and flow was checked. The used filter showed significantly lower flows than a new filter. This would lead in part to peak broadening, lower peak height and a slight lengthening of retention time. All of these effects are seen in Figure 8. At first it was assumed that this was the chief fluidic problem until closer examination revealed a leak at the input of the gas chromatographic column. This leak proved, upon testing, to be a larger source of error and contributed to the changes seen in the chromatograms. Figure 10 shows a photograph of a microfabricated gas chromatographic column with poly ether ether ketone (PEEK) fittings used to fluidically connect the column to the system. Three different PEEK fittings are also shown below the column. These three fittings were heated for increasingly longer periods of time (from left to right). Aging occurs due to temperature programming of the column during analysis. During the analysis the GC column temperature is ramped from 60°C to 120°C. Fresh epoxy is translucent whereas the aging process discolors the glue from yellow to black The fitting shown on the far right was the fitting that had the broken seal on the prototype GC column. This seal has proven to be a weak spot due to the repetitive nature of the continuous operating prototype. New seals based upon a Pyrex glass soldering process and anodic bonding are being developed.

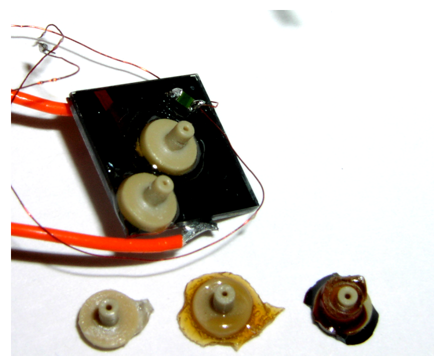

Figure 10. Aging of Microfabricated GC Column

Discussion and Conclusions

Placement of the µChemLab continuously operated prototype in the San Francisco International Airport represented the first long term unattended field test of this modified chemical analyzer. During the four-month test, over 70,000 runs were logged and the remote self-test and instrument control were exercised. The self-test hardware performed flawlessly showing no false positives. These self-tests did reveal, however, a gradual loss of signal during the tests. This loss of signal was accompanied by a shift in the chromatographic retention time for the model test compound DMMP. Post run analysis of the box revealed two sources for the drop in performance: inlet filter plugging and a pneumatic leak on the analysis GC column connection. Development efforts are underway to repair these defects and update the analyzer for future continuous operation tests.

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Appendix 1: Chemical Sensor Requirements for Facility Protection

Subway and Airport Early Warning / Situational Understanding

Requirements summary

- 24/7 monitoring
- Response time one minute or less (for initial alarm)
- Initial alarm must provide specificity between fast- and slow-acting agents
- Sensitivity at least ~30x below Incapacitating Dose/min required for subway. This is useful for airport application also, but ~300x below ICt_{50}/min is recommended
- Few false positives (<0.2/year/detector)
- No false negatives, particularly in the presence of interferents from a fire or bombing
- Concentration output for each detector with accuracy within a factor of 2 (aside from that caused by any uncertainty in agent ID)
- Accurate measurement of aerosol concentrations desired (same accuracy as for vapors). Otherwise, sensitivity at vapor pressure required.
- Self-testing capability required to confirm proper system function. (Calibrated alarms are not required.) Any released simulants must be at safe levels for release in occupied public areas.
- Remote power-on, self-test, and shut-down capability strongly recommended
- Standard 120V/60Hz AC power
- Operation in dusty environment, including very fine and metallic dust
- 6-month to one-year maintenance cycle strongly recommended (i.e. not more often). Maintenance in-place is recommended, but removal for no more than 3 days is acceptable annually.
- Serial interface for communications desired: CRC, hardware handshaking, and repeat messages upon error

More detail and additional information is included in the following sections.

Response time/Specificity

- Initial alarm in one minute or less required
  - does not require agent specificity beyond agent class, or *at least* fast- vs. slow-acting agent (for the purposes of protocols for confirmation of alarms)
  - 20-second or less response time desired, but not required
- If a second measurement can provide alarm confirmation, report within 1 to 2 minutes after initial alarm

- Agent ID desired to provide information to medical personnel within approximately 4 minutes following initial alarm. (Total time for alarm, confirmation, and ID should be less than 6 minutes if possible.)
- Concentration measurements desired every 20 seconds to support estimation of contaminated area (following initial alarm, confirmation if available, and agent ID). For detection of low concentrations at leading edge of cloud, up to two-minute cycle time is acceptable.

Sensitivity for initial alarm

~30x below ICt_{50}/min in subway; ~300x below ICt_{50}/min in airport air handlers

	Subway	**Airport**
Required		
GA, *GB, GD, GF*	1 mg/m^3 (150 ppb)	0.1 mg/m^3 (15 ppb) preferred
HD	3 mg/m^3	0.3 mg/m^3
Desired		
L, HN3	10 mg/m^3	1 mg/m^3
VX	0.3 mg/m^3	0.03 mg/m^3
AC (HCN)	30 mg/m^3	3 mg/m^3
CK (Cyanogen Chloride)	200 mg/m^3	20 mg/m^3
CG (phosgene)	50 mg/m^3	5 mg/m^3

Sensitivity for concentration mapping

Optimally, the system should provide data every 20 seconds, at 10x better sensitivity than those listed above. In order to map the plume sufficiently to predict spreading and optimally guide response, better sensitivity is desired than is strictly required for the initial alarm, so that the leading edge of the cloud can be detected in remote areas from the release. On the other hand, more frequent data is valuable for source location and plume prediction. If a trade-off is necessary between cycle time and sensitivity, a cycle time of up to 2 minutes is acceptable to achieve the desired concentrations. If these sensitivities cannot be achieved, then sensitivities up to those listed above are acceptable. Multiple operational modes are acceptable if they can be switched during operation. For example, use best sensitivity mode with response time up to 1 minute until initial alarm detected. Following initial detector alarm, alarm confirmation should be completed, if possible, within one to two minutes. Following alarm confirmation, all detectors in surrounding areas may switch to a more sensitive mode with response time up to 2 minutes. When detected concentration at a particular detector increases such that a less-sensitive faster-cycle-time mode would detect signal, switch modes to report more frequently.

False positives

< 0.2 false alarm/year/detector

(This corresponds to <~1 false alarm/month for a facility-protection system including approximately 50 detectors.)

False negatives

- Detectors must alarm in the presence of agent at the desired sensitivity, even in the presence of interferents.
- Interferents of particular interest are those that may be present if an agent is released with an explosive, or in conjunction with a fire (either for dispersal, or to confuse and harm responders). These can be approximated by testing against the following:
  - Diesel exhaust (preferably fuel rich)
  - Gasoline exhaust (preferably fuel rich)
  - Burning cardboard
  - Burning newspaper
  - Burning plastic (not required, but very good if can handle this)
- Also, since the public is present in the areas to be monitored, it would be interesting to include such things as:
  - Cigarette smoke
  - Insect repellent
  - Cleaning fluids

Temperature and Humidity

Subway 35°F to 110°F and 5% to 95% humidity
Airport air handlers: Indoor air-conditioned environment

Self-testing

Provide a method to do an end-to-end test that the system is operating properly
Provide for this test to be triggered remotely
Preferably, provide system checks with and without a small simulant release
Any simulant release must be safe for release in an occupied public area, preferably even in a small space (e.g. a subway station kiosk)

Remote Operation

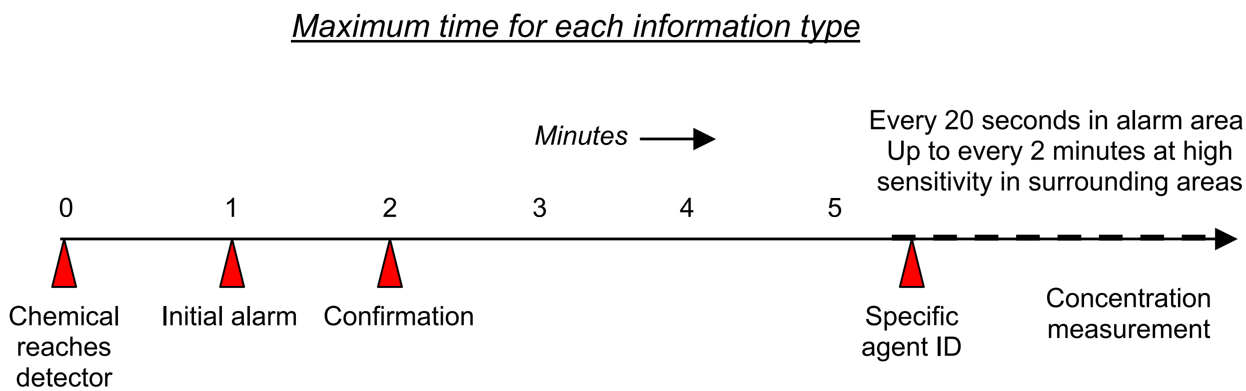
Remote control capabilities required for power-on, self-test (see above) and shutdown. For devices with multiple operating modes, remote command capability should be provided. Some mode changes, such as alarm confirmation and agent ID, where available, may be pre-programmed to follow an initial alarm. However, at a minimum, remote control will be required to return the units to the monitoring mode following an event (or unit false alarm).

Operational Example

For nominal 24/7 facility monitoring, run with one-minute response time or less.
After an initial alarm,

- switch modes for alarm confirmation within 1 minute
- switch modes for specific agent ID within 4 minutes

Thereafter, all detectors run in fastest mode that can report accurate concentrations (I.e., use slower more-sensitive mode, up to 2 minutes, if low concentration requires this for a good measurement. Switch to faster less-sensitive mode in areas of high concentration.)



Appendix 2: Flow Diagrams for the Protect Box

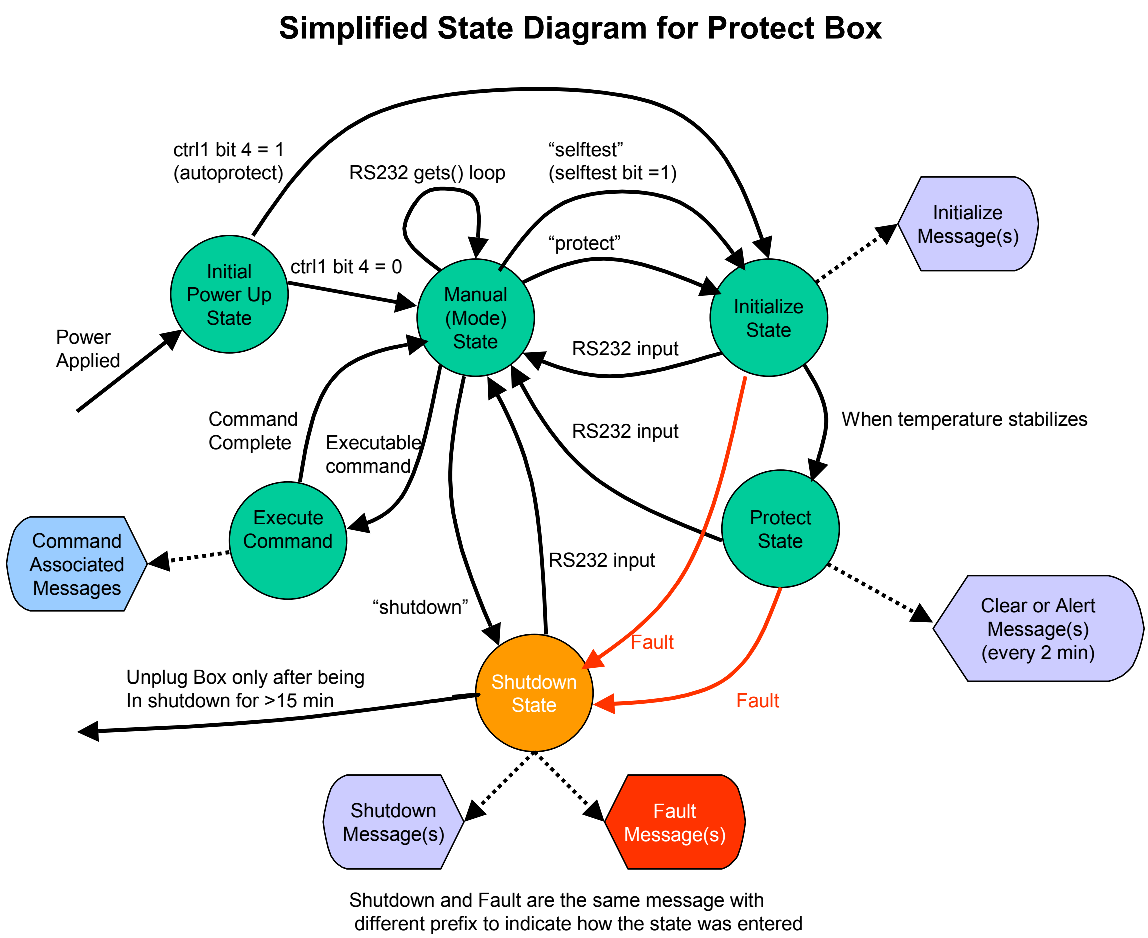


Figure 2-1: State Diagram for Sandia Continuously Operated Prototype

Protect Code – High Level View

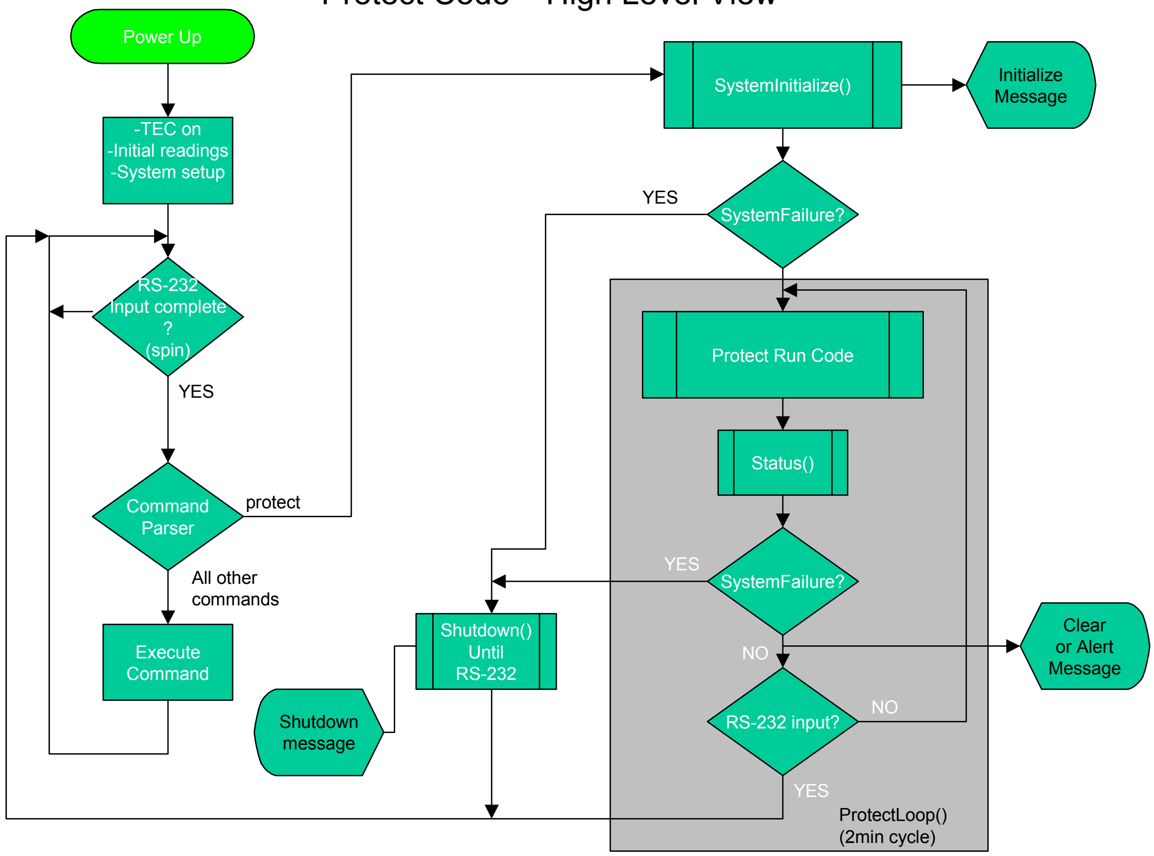


Figure 2-2: Diagram Showing Decision Tree for the Sandia Continuously Operated Prototype

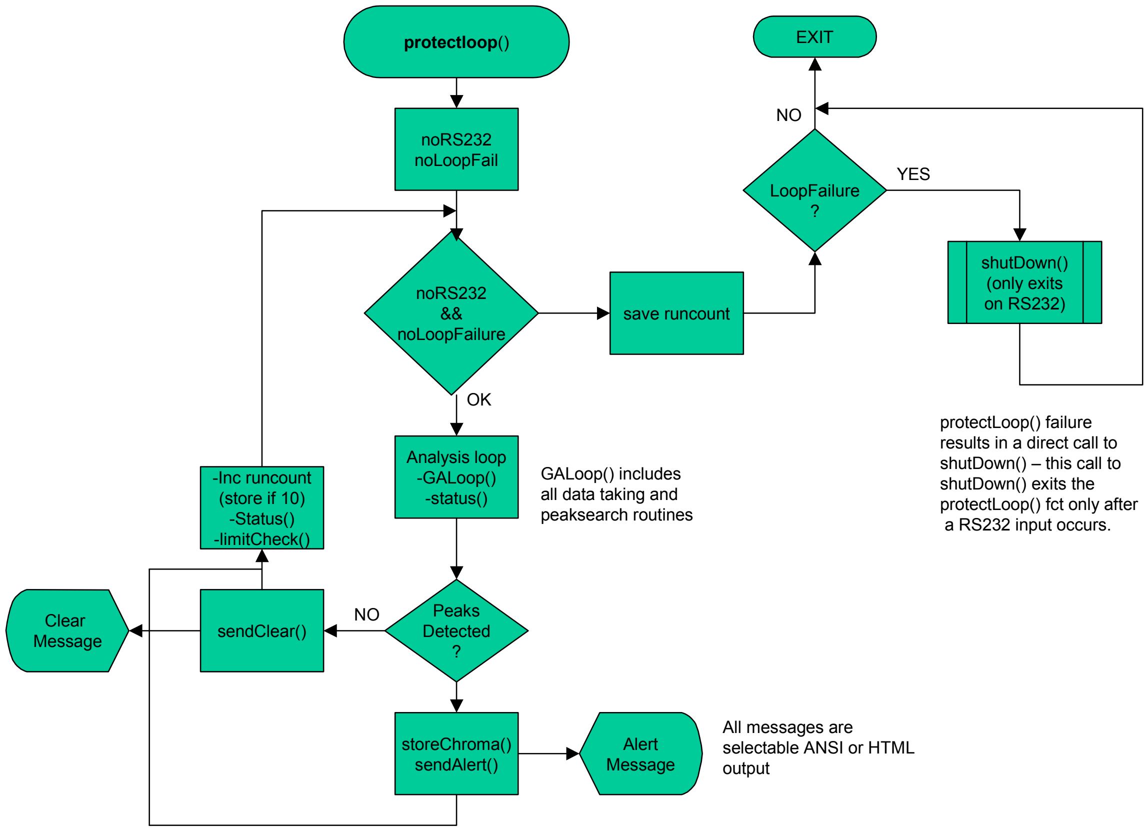


Figure 2-3: Flowchart Details for Protectloop() – Shown as Shaded Area in Figure 2-2

Appendix 3:Command Set for the Protect Box

PROTECT COMMAND SET & OPERATION- Version 2b

The command set for the PROTECT box consists of very few commands as described below. Access to the μChemLab command set is also available if the box is set to command (manual) mode. The box is set to manual by sending any character on the RS232 port.

Access to the μChemLab command set should only be done for testing or setup of the box, as these commands do not provide for autonomous operation.

The following commands will be used for PROTECT. All commands are input in ascii followed by a return -- this allows any terminal to do the control or checks. The baud rate is 38400 but may be set to 9600, 19200 or 38400. Setting the baud rate to the higher rate will allow for better downloads of stored alert data.

COMMANDS

When the PROTECT box is plugged in the first time it will enter the manual mode with no internal devices active. To make the box active you must enter "protect" after which the box will initialize. During initialization the box will issue the initialization message every 10 sec until it is ready to operate after which time "clear" or "alert" messages will be sent every 2 min. **The unit should not be left in manual mode for an extended period of time. If left unattended the unit should be put in "protect" or "shutdown".**

After initialization the box will enter the analysis mode and will issue a status message after each analysis cycle. The message will either be a "clear" message or an "alert" message (followed by an "aux" message with additional data). The user will need to "listen" for these messages continuously. **Any RS232 character sent to the unit will take the unit out of operation and put it in a command mode where individual commands can then be issued. Entering command mode may take up to 10 seconds before the command mode output line is sent. After sending a space to exit either of the operation modes (protect or shutdown) wait until the command output line is sent before proceeding with manual commands. The command line output is "*enter command or | mm for menu | protect for PROTECT*".**

When in command (manual) mode the following commands may be entered:

"**protect**" -- Box will be initialized followed by standard PROTECT run mode (issuing messages)

"**shutdown**" -- will shut down all power elements in the box except the main processor and TEC unit (to maintain temperature) "**selftest**" – will commence a selftest of the unit. This command will activate a dmmp source for one cycle and then return to the normal PROTECT run state. The unit will generate 1 to 4 (typically 2 Alerts are generated but it depends on analyte retention in system) consecutive alert messages in response to the source output. The sequence of operation is the same as "protect" but the internal source will be turned on for the first run. The initialization sequence is always run before entering the protect code loop so at least 1 initialization message will be generated.

"**mm**" – main menu. This command, given when in command mode, will display a menu of options. This command is part of the µChemLab command set.

Once the unit is put into the protect mode and has been initialized (box temp warms up to operation temperature) messages will be issued on a 2 min interval. Messages issued in "protect" are; INITIALIZATION, CLEAR, or ALERT. If a fault occurs the FAULT message will issue every 10seconds. If the unit is put in "shutdown" the unit will issue a shutdown message every 10 seconds.

CURRENT MESSAGE FORMATS

INITIALIZATION MESSAGE (during initialization after power up, if auto-protect is set, or any time protect or selftest are issued)

:INITIALIZE:SNL_P1,time,statusword,bti,hi,bto,ho,GC1,GC2,TECcp,pso,psi:

CLEAR MESSAGE (normal operation message from box)

:CLEAR:SNL_P1,time,statusword,bti,hi,bto,ho,GC1,GC2, TECcp,pso,psi,SDcount:

ALERT MESSAGE (alert message from box after detection of a target analyte)

:ALERT:SNL_P1,time,dmmp,demp,ms,SDcount:
:AUX:time,statusword ,bti,hi,bto,ho,GC1,GC2,TECcp,pso,psi:

FAULT MESSAGE (fault message occurs every 10 seconds after a fault has occurred)

:FAULT:SNL_P1,time,statusword,bti,hi,bto,ho,GC1,GC2, TECcp,pso,psi,SDcount:

SHUTDOWN MESSAGE (shutdown message occurs every 10 seconds after a shutdown has been issued). Shutdown is the same as fault but is manually initiated.

:SHUTDOWN:SNL_P1,time,statusword,bti,hi,bto,ho,GC1,GC2, TECcp,pso,psi,SDcount:

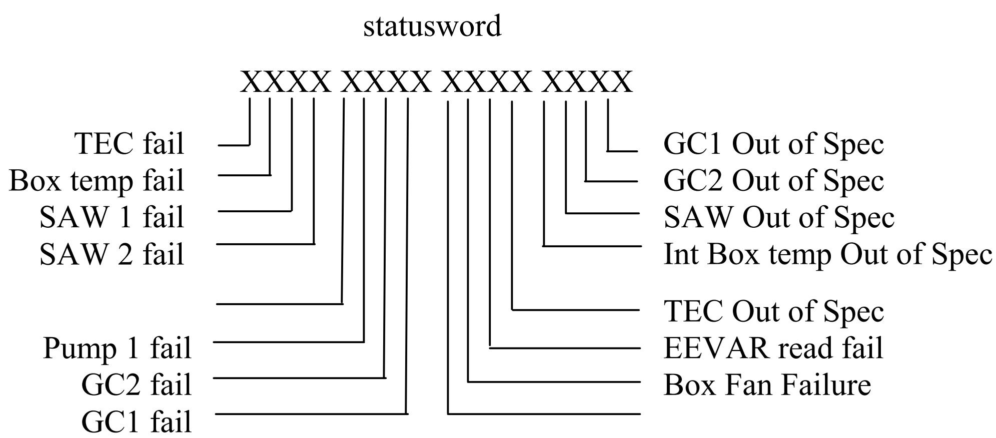
MESSAGE ARGUMENT DEFINITION

The arguments used in the message lines are defined below:

time -- time in seconds from either startup or from a preloaded number (epoch ’70 calculated value) Time may be set using “**:time:value:**” where value is in seconds.

bti, bto – box temperature - inner box, outer sample chamber, (a/d units, 0-65535)
hi, ho -- box humidity - inner box, outer sample chamber
TECcp -- TEC control point temperature (in volts x10 –> 6.09 = .609volts)
GC1,GC2 – GC temperatures (a/d units, 0-65535)

Statusword – indicates failed system or out of tolerance value. Statusword is output in hex and will be 4 characters wide. The definition is listed below.



SDcount – stored data count, number of stored alert messages/chromatographs – once this number reaches 29 it will cycle back to 0 and count up again but the last 30 chromatographs will remain stored. When reading out the data use this value as the psrd value number.

dmmp, demp, ms – outputs in ppb

OTHER COMMANDS (used from command mode)

When in command mode there are many other commands, which may be entered – so be careful what you send to the box over the RS232 channel! Most of these commands have to do with running tests on various pieces of hardware inside the box. Several commands are useful for doing basic tests and will be described here. There are two command types:

executable and colon commands. Executable commands are commands, which are run immediately after the command is issued. Some of the most useful are listed below:

bstat – outputs a line similar to some of the message lines and gives values from the same set of sensors. The output is ->

tda – stands for take data all and outputs a sequence of lines from a 6 ch a/d converter read. This will tell you in a hurry if the a/d's are running. If you get all 0's something is wrong (but see "sx" below).

sx -- sx stands for set x where x is a number of things such as a number (4,5,6,7) which power up the GC and PC circuits (good idea to leave them off since the program will operate them as required) or a letter like "o" used as "so" which stands for set oscillator and is necessary if you want to use tda above. So, the first thing to do if you try tda and get 0's for output is to do a "so" then try a tda. You should now get values for each SAW output. "ro" which stands for reset oscillator will turn the oscillator back off, again this will be handled by the program during normal runs.

dc -- dc stands for display configuration and causes several lines of configuration data to be displayed. One use for dc is to see what the current time is. Several other variables are also displayed including ctrl1 value and global indexes used to control array locations. The response to "dc" is shown below;

dc → dc is issued here
Current configuration:
time = 19134
 current channel= 3
 DeviceNum = 0
 DA num = 0
 samples = 10
 gi = 1
 gi2=40 gi3=63 gi4=15 SRDgi=15
 status1=15 status2=c0
 analysis time= 45000000
 ctrl1 = 6
 ewnum = 543
 key = A0000400
 dither = 2
 disable = 20
 fstatus = 0
 psir = 36921
 psor = 2418
 maxGCtemp = 44500

ad delay=   20
enter command or | mm for menu | protect for PROTECT → this is the standard command line

COLON COMMANDS

The other type of command is a colon command and are typically used to set EERAM stored variables (calibration coefficients and system configuration values comprise most of the values). All the colon commands start and end with a colon which the parser uses as the key to enter a subfunction which will store the variable value. Most of the colon commands are not listed here and require the use of a vapor system for calibration. Several colon commands are useful in this configuration however and are listed below.

:baud:value: -- sets the baud rate, only 3 values are possible 9600, 19200 and 38400. The default is 38400. When set, the box will switch to the new baud rate and will also come up at this baud rate on all powerups until changed again.

:time:value: -- sets the system time (in seconds). Time gets initialized at power up to a value of zero, thus you can tell how long the box has been powered. If you want to set this number to some other value, you use this command to do so, however, if you are doing this in a remote fashion then the time which is set at the box will depend on the com channel delay time.

:ctrl1:value: -- this is a control variable which controls several printout controls used through-out the box code. Most of these values will cause additional raw output from the box, which is used for calibration and general troubleshooting and should not be set. However, one switch will cause the box to come up in protect mode rather than command mode when the unit is first powered. To cause the box to come up running in protect mode use a value of 22 -> ":ctrl1:22:" . If you want to cause the unit to come up in command use a value of 6. **When installed in the field always set to 22 so that the unit will restart in the protect mode.**

:psrd:x: -- print stored results data – x is 0-29. See example below.

EXAMPLES

The first example below is output taken from the final run we did on the box (which was already warmed up so there is only a single "initialization" message) before shipping. DMMP was injected manually from the vapor system while the box was running in protect mode. This yielded the first set of ALERT messages (note that in this mode we have no control on where in the pre-concentrator collect cycle the vapor system puts out analyte, hence the first and possible last values will be different than the cal value put out by the vapor system, the 100 vs the 120 and 121 is an example of this).

DEMP (this phosphonate elutes after DMMP) was then injected which was seen as the second set of ALERT messages. Methyl Salicylate (MS) was injected and yielded the 3rd sets of ALERTS.

At the end I sent a space on the RS232 port which caused the system to exit the protect mode.

enter command or | mm for menu | protect for PROTECT
protect

:INIATIALIZE:SNL_P1, 16612, 0,41790, 3,34000, 8,32701,32660,6.06, 2480,48054:

:CLEAR:SNL_P1, 16729, 0, 41790, 4, 34400, 9,32550,32511,6.09, 2481,48155, 0:

:ALERT:SNL_P1, 16786, 100, 0, 0, 1:
:AUX:SNL_P1, 16846, 0, 41776, 3,34200, 8,40786,40696,6.07, 2481,47958:

:ALERT:SNL_P1, 16903, 120, 0, 0, 2:
:AUX:SNL_P1, 16964, 0, 41614, 2,34200, 8,40805,40697,6.05, 2478,47931:

:ALERT:SNL_P1, 17021, 121, 0, 0, 3:
:AUX:SNL_P1, 17081, 0, 41553, 3,34600, 9,40765,40713,6.09, 2482,48146:

:CLEAR:SNL_P1, 17198, 0, 41540, 3, 34200, 8,40767,40693,6.10, 2480,48063, 4:

:ALERT:SNL_P1, 17255, 0, 91, 0, 5:
:AUX:SNL_P1, 17316, 0, 41536, 3,34400, 8,40804,40708,6.05, 2480,48011:

:ALERT:SNL_P1, 17373, 0, 107, 0, 6:
:AUX:SNL_P1, 17433, 0, 41527, 3,34200, 8,40803,40695,6.07, 2481,48016:

:ALERT:SNL_P1, 17490, 0, 110, 0, 7:
:AUX:SNL_P1, 17550, 0, 41531, 3,34000, 9,40809,40729,6.04, 2482,47983:

:CLEAR:SNL_P1, 17668, 0, 41532, 3, 34000, 8,40759,40702,6.06, 2483,48117, 8:

:ALERT:SNL_P1,   17725,   0,   0, 3764,   9:
:AUX:SNL_P1,   17785,   0, 41537, 3,34000, 9,40794,40709,6.10, 2482,47972:

:ALERT:SNL_P1,   17842,   0,   0, 3509, 10:
:AUX:SNL_P1,   17903,   0, 41541, 2,34000, 8,40825,40718,6.08, 2482,47926:

:ALERT:SNL_P1,   17960,   0,   0, 3281, 11:
:AUX:SNL_P1,   18020,   0, 41540, 3,34400, 8,40804,40712,6.10, 2485,48055:

:CLEAR:SNL_P1,   18137,   0, 41535, 3, 34200, 9,40817,40718,6.04, 2481,48049, 12:

:CLEAR:SNL_P1,   18255,   0, 41538, 3, 34200, 9,40817,40655,6.06, 2483,47967, 13:

:CLEAR:SNL_P1,   18263,   0, 41537, 3, 33800, 8,40825,40721,6.08, 2482,48012, 14:

PROTECT loop has exited -- manual restart required

STORED RESULTS DATA

Below is an example of the output when stored data is read out. The colon command :psrd:2: causes the readout of stored data set #2. The first two lines are the ALERT message stored output. The raw data then follows with SAW side one (the active side) followed by SAW side 2 data. Raw data between 21 and 230 were removed from the example. The raw data consists of an index number followed by the 3 SAW channel, a/d and time data, organized as a/d1,time1 a/d2,time2,a/d3, time3. A/D channel data is in counts (0-65535) and time is in msec.
The last two lines of output are peak heights (for 3 channels) and retention time for peaks found. There will be a variable number of lines depending on number of peaks found which are at different retention times.

:psrd:2:

:ALERT:SNL_P1,   16903,   0,   121,   0,   0,   2:

:AUX:SNL_P1,   16903,   0,41614, 2,34200, 8,40805,40697,6.05, 2478,47931:

:   0:   0:   0:   0:   0:   0:   0:
:   1: 12001:   127: 51132:   131: 17907:   135:

: 2: 12000: 248: 51122: 252: 17899: 256:
: 3: 11998: 368: 51110: 373: 17893: 377:
: 4: 11999: 489: 51124: 493: 17906: 498:
: 5: 12002: 609: 51128: 614: 17911: 618:
: 6: 12001: 730: 51125: 734: 17901: 739:
: 7: 12001: 851: 51129: 855: 17906: 859:
: 8: 12002: 971: 51118: 975: 17896: 980:
: 9: 12000: 1092: 51127: 1096: 17902: 1100:
: 10: 12001: 1212: 51128: 1216: 17911: 1221:
: 11: 12006: 1331: 51135: 1336: 17910: 1340:
: 12: 11996: 1452: 51126: 1456: 17904: 1460:
: 13: 11998: 1572: 51119: 1577: 17901: 1581:
: 14: 11999: 1693: 51128: 1698: 17902: 1702:
: 15: 11995: 1814: 51118: 1818: 17904: 1823:
: 16: 12000: 1934: 51132: 1938: 17906: 1942:
: 17: 11997: 2084: 51131: 2088: 17901: 2092:
: 18: 11997: 2266: 51120: 2271: 17903: 2275:
: 19: 12001: 2449: 51128: 2454: 17906: 2458:
: 20: 12003: 2631: 51109: 2635: 17905: 2639:

: 231: 11967: 43643: 51133: 43647: 17902: 43652:
: 232: 11972: 43787: 51146: 43791: 17902: 43795:
: 233: 11967: 43931: 51132: 43935: 17908: 43939:
: 234: 11969: 44075: 51136: 44079: 17899: 44083:
: 235: 11967: 44219: 51152: 44223: 17908: 44227:
: 236: 11969: 44362: 51136: 44367: 17897: 44371:
: 237: 11968: 44506: 51146: 44510: 17906: 44515:
: 238: 11969: 44650: 51142: 44654: 17908: 44659:
: 239: 11969: 44794: 51146: 44798: 17893: 44802:
: 240: 11973: 44938: 51147: 44942: 17890: 44946:

: 0: 0: 0: 0: 0: 0: 0:
: 1: 9777: 187: 46817: 191: 49628: 195:
: 2: 9782: 307: 46820: 312: 49618: 316:
: 3: 9783: 428: 46812: 432: 49621: 437:
: 4: 9781: 548: 46805: 553: 49615: 557:
: 5: 9780: 669: 46799: 673: 49622: 678:
: 6: 9783: 790: 46821: 794: 49629: 798:
: 7: 9780: 910: 46803: 914: 49624: 919:
: 8: 9786: 1031: 46823: 1035: 49617: 1039:
: 9: 9779: 1151: 46810: 1155: 49620: 1160:
: 10: 9785: 1272: 46818: 1276: 49623: 1280:
: 11: 9780: 1391: 46809: 1395: 49622: 1399:
: 12: 9782: 1511: 46816: 1516: 49630: 1520:

:   13: 9781: 1632: 46822: 1637: 49622: 1641:
:   14: 9778: 1753: 46810: 1757: 49628: 1761:
:   15: 9786: 1874: 46813: 1878: 49616: 1882:
:   16: 9780: 1993: 46798: 1997: 49632: 2002:
:   17: 9776: 2174: 46826: 2179: 49616: 2183:
:   18: 9786: 2356: 46828: 2362: 49621: 2366:
:   19: 9783: 2540: 46822: 2544: 49620: 2548:
:   20: 9781: 2721: 46826: 2725: 49634: 2730:

: 231: 9784: 43726: 46802: 43730: 49611: 43734:
: 232: 9779: 43870: 46813: 43874: 49615: 43878:
: 233: 9778: 44013: 46795: 44018: 49609: 44022:
: 234: 9780: 44158: 46808: 44162: 49618: 44166:
: 235: 9778: 44301: 46824: 44306: 49628: 44310:
: 236: 9780: 44445: 46805: 44449: 49618: 44454:
: 237: 9780: 44589: 46813: 44593: 49620: 44598:
: 238: 9781: 44733: 46802: 44737: 49620: 44741:
: 239: 9779: 44877: 46810: 44881: 49627: 44885:
: 240: 9783: 45020: 46810: 45025: 49620: 45029:
:   335:   20:   13: 5179:
no peaks found on SAW2
enter command or | mm for menu | protect for PROTECT

Distribution

5	MS0892	Richard Kottenstette, 1764
1	MS0892	Patrick Lewis, 1764
1	MS0892	Douglas Adkins, 1764
1	MS0892	Richard Cernosek, 1764
1	MS1073	George Dulleck, 1738
1	MS1073	Michael Daily, 1738
1	MS1425	Stephen Martin, 1707
1	MS1077	Thomas Zipperian, 1740
1	MS1079	Marion Scott, 1700
1	MS9201	Susanna Gordon, 8112
1	MS9201	Greg Foltz, 8112
1	MS9201	Bill Wilcox,8112
1	MS9951	Art Pontau, 8358
1	MS9951	Duane Lindner, 8101
1	MS9405	John Vitko, 8001
1	MS9018	Central Technical Files, 8945-1
2	MS0899	Technical Library, 9616
1	MS0612	Review and Approval Desk, 9612 For DOE/OSTI